Tutorial: Brain Network Analysis with Graph Neural Networks

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ABSTRACT

Mapping the connectome of the human brain using structural or functional connectivity has become one of the most pervasive paradigms for neuroimaging analysis. Recently, Graph Neural Networks (GNNs) motivated from geometric deep learning have attracted broad interest due to their established power for modeling complex networked data. Despite their superior performance in many fields, there has not yet been a systematic tutorial on practical GNNs for brain network analysis. In this tutorial, we will cover (1) the summarization of brain network construction pipelines for both structural and functional neuroimaging modalities; (2) the modularization of fundamental GNN designs for brain networks and a set of recommendations on general effective recipes based on empirical observations; (3) hands-on instructions on our out-of-box Python package BrainGB, which is available at https://braingb.us with models, tutorials, and examples; (4) more advanced GNN designs and training strategies for brain network analysis and future directions. We believe this tutorial can bridge researchers in neuroscience and machine learning/deep learning and offer insights for future research in this novel and promising direction.

KEYWORDS

Brain network analysis, graph neural networks, deep learning for neuroscience, medical imaging

1 TARGET AUDIENCE AND PREREQUISITES

The target audience for this tutorial includes researchers, engineers, or graduate students in the field of computational neuroscience, brain network analysis, or machine learning as well as those who are new to the topic or who are interested in this topic. The audience is expected to have a basic understanding of machine learning and deep learning. Prior knowledge of Graph Neural Networks (GNNs), graph theory, and neuroimaging data analysis would be beneficial but not essential, as the tutorial aims to provide an overview of the techniques and their applications in brain network analysis. Some experience with programming and popular deep learning frameworks such as PyTorch would also be helpful in following the hands-on section and understanding the implementation details.

2 PRESENTER BIOGRAPHY

Hejie Cui is a fourth-year Ph.D. candidate in Computer Science at Emory University, working with Prof. Carl Yang in Emory Graph Mining Lab. Her research interests span Graph Data Mining, Graph Neural Networks, Knowledge Graphs, Multi-modal Learning for Text and Images/Videos, as well as their applications in Neuroscience and Healthcare. Hejie has published/co-authored several papers on top venues including NeurIPS, KDD, AAAI, CIKM, MICCAI, ECML, SDM, ECIR, etc. She is also a recipient of the Fellowship of 2021 CRA-WP Grad Cohort for Women in 2021, the Student Travel Grant Award for MICCAI2022, and the NSF Travel Grant for CIKM2022. She participated in organizing the first International Workshop on Neural Network Models for Brain Connectome Analysis (BrainNN2022) at IEEE BigData.

Xuan Kan is a fourth-year Ph.D. candidate in Computer Science at Emory University, under the joint supervision of Prof. Carl Yang and Prof. Ying Guo. Previously, he obtained his B.Eng. in Software Engineering from Tongji University. His research focuses on designing machine learning algorithms that are both efficient and interpretable for fMRI data, with the goal of aiding neurobiological research and facilitating the diagnosis of mental diseases. Xuan has published multiple papers on functional brain network analysis in top-tier conferences such as NeurIPS, KDD, ISBI, and MIDL, and has played a role in organizing the BrainNN2022.

Xiaoxiao Li is an Assistant Professor in the Electrical and Computer Engineering Department and an Associate Member in the Computer Science Department at the University of British Columbia (UBC), leading the Trusted and Efficient AI (TEA) Lab. She is also a core faculty member of Blockchain@UBC, a member of Biomedical Imaging and Artificial Intelligence, and a member of LEAP project. Starting from 2022, She is an adjunct Assistant Professor at Yale University. Before joining UBC, she was a postdoc in the Department of Computer Science at Princeton, working with Prof. Kai Li and Prof. Olga Troyanskaya. She obtained her Ph.D. degree in Biomedical Engineering from Yale University advised by Prof. James Duncan, with Yale Advanced Graduate Leadership Fellowship. Her current research lies in machine learning and its application to healthcare and blockchain.

Lifang He is an Assistant Professor in the Department of Computer Science and Engineering at Lehigh University. She received the B.S. degree in Computational Mathematics from Northwest Normal

University, and the Ph.D. degree in Computer Science from South China University of Technology. Before joining Lehigh's faculty, she was a postdoctoral associate in the Department of Biostatistics, Epidemiology and Informatics within the Perelman School of Medicine at the University of Pennsylvania, and the Weill Cornell Medical College of Cornell University. Her research is focused on developing new machine learning methods for solving challenging problems in biology and biomedicine, and ultimately furthering the understanding of disease pathologies and improvement of treatment strategies. Dr. He has worked extensively on the development of innovative methods for brain connectome analysis and has a long history of successful interdisciplinary collaborations with researchers in neuroscience and biology.

Liang Zhan is an Associate Professor in the Department of Electrical & Computer Engineering and Bioengineering at the University of Pittsburgh, where he also serves as the associate director of the Pittsburgh Center for Artificial Intelligence Innovation in Medical Imaging (CAIIMI). His research areas include brain connectomics and data mining, as well as clinical/translational research on brain diseases, such as Alzheimer's disease, Parkinson's disease, bipolar disorder, depression, and Traumatic Brain Injury, etc. He has extensive experience with graph neural network models for brain network data. He received his PhD from the University of California, Los Angeles (UCLA) in 2011. Besides NSF Career award, his research is supported by NIH R21, R01s, U01, NSF IIS, and OIS, as well as US Department of Veterans Affairs.

Ying Guo is a Professor in the Department of Biostatistics and Bioinformatics at Emory University, an appointed Graduate Faculty of the Emory Neuroscience Program and an Associate Faculty in Emory Department of Computer Science. She is a Founding Member and current Director of the Center for Biomedical Imaging Statistics (CBIS) at Emory University. Dr. Guo's research focus on developing analytical methods for neuroimaging and mental health studies. Her main research areas include statistical modeling and learning for agreement and reproducibility studies, brain network analysis, multimodal neuroimaging, hierarchical modeling and imaging-based prediction. Dr. Guo has served on the Editorial Boards of Biometrics, Statistics in Biosciences and Psychosomatic Medicine. She is a Fellow of American Statistical Association (ASA) and Chair-Elect of the ASA Statistics in Imaging Section. Dr. Guo has served as the principal investigator on several NIH R01 awards and she is a Standing Member of NIH Emerging Imaging Technologies in Neuroscience (EITN) Study Section.

Carl Yang is an Assistant Professor in Emory University. He received his Ph.D. in Computer Science at the University of Illinois, Urbana-Champaign and B.Eng. in Computer Science and Engineering at Zhejiang University. His research interests span graph data mining, applied machine learning, knowledge graphs and federated learning, with applications in recommender systems, biomedical informatics, neuroscience and healthcare. Carl's research results have been published in top venues like TKDE, KDD, WWW, NeurIPS, ICML, ICLR, ICDE, SIGIR and ICDM. He also received the Dissertation Completion Fellowship of UIUC in 2020, the Best Paper Award of ICDM in 2020, the Best Paper Award of KDD Health Day in 2022, the Outstanding Paper Award of ML4H in 2022, the Amazon Research Award and multiple Emory internal research awards.

3 TUTORIAL DESCRIPTION

The human brain is at the center of complex neurobiological system that controls behavior and cognition. Brain imaging studies have found that interactions between brain regions play a key role in neural development and disorder analysis [9, 19]. Brain networks, modeled using graph theory, describe the interactions between brain regions. Medical imaging techniques such as MRI are used to scan the brain, which is the most widely used for brain analysis research. Different MRI modalities, like fMRI and DTI, can be used to construct functional and structural brain networks, which describe correlations between brain regions and physical connections between gray matter regions [27], respectively. These connections are valuable resources for understanding the brain [4, 24].

Previous studies on brain network analysis used shallow models based on graph theory [4, 32] and tensor factorization [22, 41] to detect network communities and identify central elements, but these models can be limited to complex brain network structures [10]. In recent years, Graph Neural Networks (GNNs) have attracted broad interest in analyzing graph-structured data [17, 34, 36]. Several pioneering deep models have been devised to predict brain diseases by learning graph structures of brain networks. For instance, Li et al. [19] propose BrainGNN to analyze fMRI data, where ROI-aware graph convolutional layers and ROI-selection pooling layers are designed for neurological biomarker prediction. Kawahara et al. [15] design a CNN framework BrainNetCNN composed of edge-to-edge, edge-to-node, and node-to-graph convolutional filters that leverage the topological locality of structural brain networks. However, due to the ethical issue of human-related research, the datasets used are usually not publicly available and the details of imaging preprocessing are not disclosed, rendering the experiments irreproducible for other researchers. Besides, training deep models requires large amounts of labeled data, which is often scarce in brain network datasets due to the complexities of data acquisition.

To address these aforementioned problems, recently researchers have widely leveraged different machine-learning techniques for GNN-based brain network analysis, including interpretable model designs [5, 6, 8, 14, 19], multimodality analysis [23, 42], dynamic network analysis [16, 20], generative neural networks [13, 40], resource-limited training [38, 39], etc. In this tutorial, we systematically review and discuss the recent advances in brain network analysis with Graph Neural Networks (GNNs), and provide a hands-on tutorial section for researchers from inter-disciplined areas who are interested but new to the field. In both the neuroscience and graph machine learning community, we believe that is an edge-cutting research topic with important scientific impacts, and can potentially inspire new understanding or innovative ideas for neural network designs.

4 TUTORIAL OUTLINE

- **Introduction and Overview**
  In this section, we will introduce the background knowledge about brain network data and Graph Neural Networks (GNNs). Afterward, we will discuss the challenges of effectively adopting GNNs for brain network analysis:
  - Brain Network Analysis [7, 12, 21, 25, 26, 30, 31, 37]
  - Graph Neural Networks [17, 29, 36]

  - Challenges of GNNs for Brain Network Analysis [3, 5, 19, 33]
- **Brain Network Construction**
  In this section, we will discuss the diverse modalities of neuro-imaging [28] and illustrate the main procedures to construct brain networks that model different connectivity (i.e., functional or structural) from popular modalities of raw neuro-imaging data [11, 18, 21, 31]:
  - Functional Brain Network Construction [35, 35]
  - Structural Brain Network Construction [1, 2]
- **Fundamental GNN Design for Brain Network Analysis**
  In this section, we decompose the design space for basic message-passing GNN design into four modules and explain different possible variants under each dimension, together with the empirical insights on general recipes for effective GNN designs on brain networks, which is all integrated into our BrainGB [5] package and serve as a starting point for further studies:
  - Node Feature Construction
  - Message Passing Mechanisms
  - Attention-Enhanced Message Passing
  - Pooling Strategies
- **BrainGB Package Hands-on**
  In this section, we will provide hands-on instructions on the out-of-box package BrainGB on an example brain network dataset. The instruction materials are available at https://braingb.us.
- **Advanced GNN Designs for Brain Network Analysis**
  In this section, we cover a series of advanced GNN designs and training strategies for brain network analysis, including
  - GNN for Multimodality Brain Networks [23, 42]
  - Interpretable GNN for Brain Networks [6, 8, 14, 19]
  - GNN for Dynamic Brain Networks [16, 20]
  - Generative GNN for Brain Networks [13, 40]
  - Resource-limited GNN Training for Brain Networks [38, 39]
- **Discussions and Future Directions**
  At last, we will elucidate open challenges and future directions from the following perspectives:
  - Neurology-driven GNN design
  - Pre-training and transfer learning of GNNs for Brain Networks

5 ADDITIONAL INFORMATION

5.1 Related Tutorials

As per our knowledge, there is no existing tutorial exactly on brain network analysis with graph neural networks, although both directions of brain network analysis and graph neural networks have their own tutorials. For brain network analysis, (1) Maria Giulia Preti, EPFL, Switzerland and Thomas Bolton, Graph Signal Processing Opens New Perspectives for Human Brain Imaging, at ISBI 2022; (2) Eduarda Gervini Zampieri Centeno, Giulia Moreni, Chris Vriend, Linda Douw, and Fernando Antônio Nóbrega Santos, A hands-on tutorial on network and topological neuroscience, at Brain Structure and Function (Brain Struct Funct) 2021; (3) Bernard Ng, Sanmi (Oluwasanmi) Koyejo, and Sandro Vega Pons, Brain Network Analysis, at Pattern Recognition in Neuroimaging (PRNI) 2016; (4) Danielle S. Bassett, Brain network analysis: a practical tutorial at Brain 2016. Although these listed tutorials cover brain network analysis in both theoretical and practical manners, none of them focus on the recent emerging graph neural network and stress the issue of insufficient training data for deep models.

For graph neural networks, there are plenty of tutorials on GNN models which cover various applications and challenging settings, such as (1) Lingfei Wu, Peng Cui, Jian Pei, Liang Zhao, and Xiaojie Guo, Graph Neural Networks: Foundation, Frontiers and Applications, at KDD 2022; (2) Kaize Ding, Chuxu Zhang, Jie Tang, Nitesh Chawla, and Huan Liu, Toward Graph Minimally-Supervised Learning, at KDD 2022; (3) Jian Kang and Hanghang Tong, Algorithmic Fairness on Graphs: Methods and Trends, at KDD 2022; (4) Wei Jin, Yao Ma, Yiqi Wang, Xiaorui Liu, Jiliang Tang, Yukuo Cen, Jiezhong Qiu, Jie Tang, Chuan Shi, Yanfang Ye, Jiawei Zhang, and Philip S Yu, Graph Representation Learning: Foundations, Methods, Applications and Systems, at KDD 2021; (5) Xin Wang and Wenwu Zhu, Automated Machine Learning on Graph, at KDD 2021. We do not illustrate the details of each of them here. Besides, there is a tutorial on more general geometric deep learning on imaging data: Jelmer Wolterink, Angelica I Aviles-Rivero, and Erik Bekkers, GeoMedIA: Geometric Deep Learning in Medical Image Analysis, at MICCAI 2022, which covers neural networks for learning on point clouds, graphs, and meshes.

5.2 Participation and Interactivity

During the tutorial, we plan to incorporate interactive activities such as group discussions and question-and-answer sessions, along with lectures to keep the audience engaged and involved in the learning process. These activities will provide opportunities for the audience to share their own experiences, ask questions, and discuss real-life scenarios related to the topic. We also plan to use visual aids, such as slides and diagrams, to support the lecture content and make the information easier to understand. Furthermore, we will encourage the audience to bring their laptops to participate in the hands-on sessions, where they can apply what they have learned and gain practical experience. We will also post all the materials of this tutorial, including tutorial documents, presentation slides, and speaker recorders for post-tutorial reviews.

5.3 Potential Impact

This tutorial has the potential to have a significant impact on the field of computational neuroscience and deep learning. By providing a comprehensive overview of brain network analysis with Graph Neural Networks (GNNs), it can help researchers, practitioners, and students understand the latest deep geometric learning techniques and use them for brain network analysis. The hands-on sessions and real-world case studies can help the participants apply their newfound knowledge to their research, leading to more efficient verification. Moreover, the tutorial can also foster collaboration and knowledge sharing among participants from different disciplines, which leads to innovative approaches to analyzing brain networks and contribute to the advancement of this field.

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